Occurrence of an Anomalous Cu 2p HAXPES Peak in Electron-Doped Nd_2CuO_4

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One of the most remarkable findings in recent hard X-ray photoemission spectroscopy (HAXPES) is the occurrence of an anomalously strong Cu 2p XPS peak in electron-doped Nd_2CuO_4 (NCO) measured by Taguchi et al.[1] The experimental results of Cu $2p_{3/2}$ XPS of $Nd_{1.85}Ce_{0.15}CuO_4$ are shown in the inset of Fig.1, where the anomalous peak α was revealed in HAXPES (indicated by HX) but was almost absent in soft X-ray photoemission measurements (indicated by SX). Taguch et al. interpreted that this new peak originates from the metallic screening effect based on phenomenological model calculations, where an extra electronic level representing the doped-electron states is combined with the single impurity Anderson model describing an undoped system. In the present paper, we calculate Cu 2p XPS, by extending our previous paper [2], for both doped and undoped NCO by exact diagonalization method for multi-Cu-site cluster model, where the effect of electron-doping is naturally treated without introducing by hand an extra electronic level. We show in Fig.1 an example of the calculated Cu 2p XPS for 16.6 % electron-doped NCO with a Cu_6O_{17} cluster model (see the upper panel of Fig.1). The solid and chain curves are obtained by the Lorentzian convolution widths 1.0 eV and 0.2 eV, respectively. We can show that the anomalous peak α is caused by the metallic screening effect, in agreement with the interpretation by Taguchi et al., but now based on the more direct and more microscopic calculations. For Cu 2p XPS of undoped NCO, on the other hand, our calculation shows clearly the existence of the Zhang-Rice singlet feature, in contrast that Taguchi et al.[1] claimed the absence of this feature.

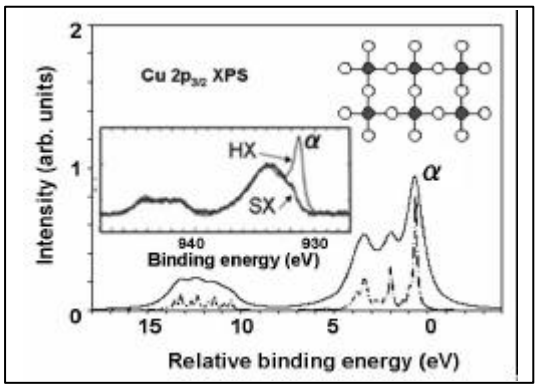

Fig. 1

[1] M. Taguchi et al., Phys. Rev. Lett. **95**, 177002 (2005).
[2] K. Okada and A. Kotani, J. Phys. Soc. Jpn., 74, 653 (2005).